

Ethyl phenylacetate
101-97-3 | DTXSID6044353

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.52

Global applicability domain: Inside

Local applicability domain index: 7.06e-01

Confidence level: 8.00e-01

Nearest Neighbors from the Training Set

Image not found

Benzenepropanoic acid, methyl ester

Measured: 2.32

Predicted: 2.52

Image not found

Ethyl phenylacetate

Measured: 2.28

Predicted: 2.52

Image not found

Methyl 2,6-dimethylbenzoate

Measured: 2.55

Predicted: 2.31

Image not found

Methyl 2-methylbenzoate

Measured: 2.75

Predicted: 2.51

Image not found

Benzoic acid, 3-methyl-, methyl ester

Measured: 2.77

Predicted: 2.55